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Stable Topological Skyrmions on the 2D Lattice.

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Abstract. In the continuum O(3) sigma model in two spatial dimensions, there are topological solitons whose size can be stabilized by adding Skyrme and potential terms. This paper describes a lattice version, namely a natural way of modifying the 2d Heisenberg model to achieve topological stability on the lattice.

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1. Introduction.

Topological solitons in sigma models, and specifically in the two-dimensional O(3) sigma model, have been studied in several different contexts:

- as metastable states in two-dimensional ferromagnets [1,2];
- as instantons in a field theory which models four-dimensional gauge theory [3];
- as a model for particles, in particular as a simpler version of the three-dimensional skyrme model [4,5].

In each of these applications, the lattice version of the model (where the field is defined on a two-dimensional lattice), is relevant. For condensed-matter applications, the relevance is direct; while for field-theory applications, a discrete version is needed in order to do numerical computations [6,7,8,9,4,5]. In the usual lattice version of the O(3) sigma model, namely the Heisenberg model, the topological properties are essentially lost (which is what one would expect, since topology has to do with continuity). But in this paper we shall see how topology (and topological stability of the solitons) can be maintained on the lattice.

2. A Topological Heisenberg Model.

Let L be an $n_x \times n_y$ lattice; in other words, there are $n_x n_y$ lattice sites, labelled by integers (x, y) with $1 \le x \le n_x$ and $1 \le y \le n_y$. The field φ is a map from L to S^2. Think of $\varphi_{x,y}$, the field (or spin) at the lattice site (x, y), as a three-dimensional unit vector. The energy of φ is defined by the expression

$$\begin{aligned} E = \frac{1}{4\pi} \sum_{x=1}^{n_x-1} \sum_{y=1}^{n_y} f(\varphi_{x,y} \cdot \varphi_{x+1,y}) + \frac{1}{4\pi} \sum_{x=1}^{n_x} \sum_{y=1}^{n_y-1} f(\varphi_{x,y} \cdot \varphi_{x,y+1}) \\ + \frac{\mu^2}{4\pi} \sum_{x=1}^{n_x} \sum_{y=1}^{n_y} (1 - \varphi_{x,y} \cdot k). \end{aligned} \tag{1}$$

Here f is a real-valued function with $f(1) = 0$ and $f'(1) = -1$, the dot denotes the Euclidean scalar product, μ is a constant scalar, and k is a constant unit vector.

First, let us examine the continuum limit. To this end, let n_x and n_y be infinite, introduce a lattice spacing h (so that x and y temporarily become integer multiples of h), and replace μ by $\tilde{\mu} = \mu/h$. Then the $h \to 0$ limit of (1) is

$$E_{\text{cont}} = \frac{1}{4\pi} \int_{\mathbf{R^2}} \left[\tfrac{1}{2} (\partial_x \varphi)^2 + \tfrac{1}{2} (\partial_y \varphi)^2 + \tilde{\mu}^2 (1 - \varphi \cdot k) \right] dx\, dy. \tag{2}$$

If $\tilde{\mu} = 0$, this is the two-dimensional O(3) sigma model; the $\tilde{\mu}$ term is an optional potential. Notice that the function f does not appear in (2): any f which is smooth near 1, with $f(1) = 0$ and $f'(1) = -1$, leads to (2).

The boundary condition is $\varphi \to k$ as $r \to \infty$ on $\mathbf{R^2}$ (sufficiently fast for $E_{\rm cont}$ to converge). The configuration space of smooth fields φ satisfying this boundary condition is disconnected: its components are labelled by an integer N, the winding number or topological charge of φ. A version of the Bogomol'nyi argument gives a topological lower bound on $E_{\rm cont}$, namely

$$E_{\rm cont} \geq |N| \tag{3}$$

(see, for example, [3]). If $\tilde{\mu} = 0$, then there are fields which saturate (3), and which are therefore automatically solutions of the sigma-model field equations [1,2]. These solutions look like localized "solitons" in $\mathbf{R^2}$. Roughly speaking, these solitons are located at the (isolated) points where $\varphi = -k$, ie. where the field is antipodal to its boundary value. But because of the scale invariance of (2) when $\tilde{\mu} = 0$, the size of the solitons is not fixed. So a perturbation of a soliton can cause it to become arbitrarily concentrated or spread out. That this indeed happens is confirmed by numerical experiment [9].

One way of stabilizing the soliton is to put in the $\tilde{\mu}$ term, which prevents spreading out; and also to add to $E_{\rm cont}$ a Skyrme term

$$E_{\rm Skyrme} = \frac{1}{4\pi} \int_{\mathbf{R^2}} \tfrac{1}{2} (\partial_x \varphi \wedge \partial_y \varphi)^2 \, dx \, dy, \tag{4}$$

which prevents shrinkage [10,4,11,12,5]. The opposing effects of the $\tilde{\mu}$ and Skyrme terms fix the size of the soliton (now called a skyrmion) to be of order $\tilde{\mu}^{-1}$, in the sense that its profile contains a factor $\exp(-\tilde{\mu} r)$. If $\tilde{\mu}^2 = 0.1$, then the energy of the $N = 1$ skyrmion equals 1.564, i.e. about 50% higher than the energy of the basic $N = 1$ sigma-model soliton [12,5]. This skyrmion is stable against any perturbation which maintains the boundary condition and topological charge. Such perturbations can have arbitrarily large energy, and this represents a very high degree of stability.

Let us return now to the lattice case (1). We impose the boundary condition that $\varphi = k$ on the boundary of the lattice (or $\varphi \to k$ if the lattice is infinite, in which case the condition is necessary to ensure finite energy). For the time being, put $\mu = 0$.

The standard Heisenberg model is obtained by taking $f(\xi) = 1 - \xi$. In this case, there is no topology; the configuration space is a connected manifold. If we remove (by hand) some

"exceptional" configurations, then the resulting space does have disconnected components labelled by an integer N, corresponding to the topological sectors of the continuum case [6]. But if one tries to minimize the energy E within a nontrivial sector (say $N = 1$), then one is driven towards an exceptional configuration [7]. Another way of putting this is that if one sets up an initial field which looks like a soliton (ie. $\varphi \approx -k$ at some interior lattice sites), then it tends to shrink and "unwind", and is certainly not stable. This feature also appears in numerical simulations of the continuum sigma model, which in effect involves replacing the continuum by a lattice [9].

In the continuum, a soliton can be prevented from shrinking by the presence of the Skyrme term (4). The obvious lattice analogue of this involves next-to-nearest-neighbour couplings between lattice sites, in addition to the nearest-neighbour couplings appearing in (1). One model along these lines was discussed in [8]. This involved adding certain second- and third-nearest neighbour couplings. With an appropriate tuning of parameters, the lattice skyrmion then becomes stable (a curious feature is that these more distant couplings need to be opposite in sign to the nearest-neighbour ones). But this stability is rather delicate (certainly far weaker than the topological stability of the continuum skyrmions). A fairly small perturbation can induce these lattice skyrmions to decay.

The basic reason for the instability, and the absence of topology, is that there is nothing to prevent neighbouring spins from being wildly different. In the Heisenberg model it is energetically favourable for a soliton to shrink to the size of a single lattice cell, in the sense that the spins $\varphi_{x,y}$, $\varphi_{x+1,y}$, $\varphi_{x,y+1}$, $\varphi_{x+1,y+1}$ at the four corners of this cell lie on a great circle in the image sphere S^2. This is an "exceptional configuration", and from it the field rapidly unwinds. Clearly in this exceptional configuration there is at least one pair of neighbouring spins which differ by an angle of at least $\pi/2$. Conversely, if we could ensure that the angle between neighbouring spins was always acute, then unwinding could not occur, and topology would be restored. Such a model is the subject of this paper, and will now be described.

The idea is to take $f(\xi)$ to be a function which tends to infinity as $\xi \to 0$, for example

$$f(\xi) = -\log(\xi). \tag{5}$$

Then if we start with an initial configuration in which the angle between neighbouring spins is less than $\pi/2$, the field cannot evolve into one which violates this acuteness condition.

If the angle between a pair of neighbouring spins is θ, then the force which tries to align the spins (ie. reduce θ) is proportional to $\tan\theta$; so θ can never reach $\pi/2$. By contrast, the analogous force in the Heisenberg model goes like $\sin\theta$.

In the condensed-matter context, the choice (5) is unphysical. A more physical choice would be one which increases the energy penalty on pairs of spins which deviate too much, without involving infinite forces. For example, one could take

$$f(\xi) = (1-\xi) + c(1-\xi)^2, \tag{6}$$

where c is a large positive constant. Such models have indeed been studied in condensed-matter physics. But they are not topological in the sense of this paper, and so we shall use (5) in what follows. However, one might expect that (5) and (6) give solitons with similar properties (under appropriate conditions). Of course, they have the same continuum limit, namely the sigma model (2).

The configuration space now consists of all fields φ such that the angle between any pair of neighbouring spins is less than $\pi/2$. The energy E is given by (1), with (5), and is a well-defined positive-definite function. The configuration space is disconnected, with components labelled by an integer N; an algorithm for computing N may be found in [6]. If we start in the Nth topological sector and allow the field to evolve, then it has to remain in this sector: there are infinite potential barriers between the sectors. And in any given sector there must exist one or more stable solitons, ie. fields which minimize E.

3. Numerical Results on Lattice Solitons.

Our task in this section is to find the minimum-energy configurations of charges $N = 1$ and $N = 2$. This involves minimizing a function of $2(n_x - 2)(n_y - 2)$ variables, and has to be done numerically. The minimization is done in two steps. The first step is to assume a "radial symmetry" with exponentially-decaying profile $g(r) = \pi\exp(-br)$, and to find the value of b which minimizes the energy E (more details are given below). In other words, we reduce to a function of the single variable b and minimize over that. In fact, this gives a field which is quite close to the true minimum. The second step is to take this approximation as a starting-point, and minimize over all the degrees of freedom, obtaining the minimum-energy field to the desired level of accuracy. This is done by using a conjugate gradient method.

The details of the radial approximation are as follows. The quantity

$$r = \sqrt{(x - \tfrac{1}{2}n_x - \tfrac{1}{2})^2 + (y - \tfrac{1}{2}n_y - \tfrac{1}{2})^2}$$

measures the distance from the centre of the lattice to the site (x, y). The 3-vector φ is taken to be

$$\varphi = \big(r^{-1}(x - \tfrac{1}{2}n_x - \tfrac{1}{2})\sin g(r), r^{-1}(y - \tfrac{1}{2}n_y - \tfrac{1}{2})\sin g(r), \cos g(r)\big), \tag{7}$$

except on the boundary of the lattice where it equals $k = (0, 0, 1)$. Substituting (7) into (1) gives E as a function of b, and this is then minimized.

Let us first deal with (and dispose of) the case $\mu = 0$. On the continuous plane $\mathbf{R^2}$, the μ-term is necessary to prevent the skyrmion from spreading out indefinitely; and the same is true on the infinite lattice. To be more precise: if we take a square lattice with $n_x = n_y = n$, then the size of the $N = 1$ skyrmion grows like $n/3$ for large n. Here "size" means twice the radius; and the radius is taken to be the distance from the centre at which the third component of φ reaches the value of 0.95 (it equals 1 at the boundary). So the skyrmion is only prevented from expanding indefinitely by the boundary of the lattice. Conversely, if we want a skyrmion whose behaviour is not affected by the boundary, then we have to stabilize its size by taking μ to be positive. From now on, this is what we shall do.

By analogy with the continuum case, one might expect the size of a skyrmion (in the absence of boundary effects) to be proportional to μ^{-1}. This is indeed the case. One finds numerically that the size grows like $\frac{2}{3}\mu^{-1}$, for μ^{-1} large (compared to unity). From now on, μ^{-1} is set equal to 2. Then the size of the 1-skyrmion is 7 lattice-units; and as long as n_x and n_y are greater than 20, boundary effects are negligible. To be more precise, changing the size of the lattice affects the value of the (minimized) energy by less than one part in 10^5, and this is the level of accuracy in what follows.

Taking $n_x = n_y = 22$, we get a minimum energy of $E = 1.57985$. The corresponding field is depicted in figure 1. What is plotted there (and in all the other figures) is energy density as a function of x and y. So the horizontal grid represents the lattice, and and we are plotting the quantity

$$\begin{aligned} &-\frac{1}{8\pi}\log(\varphi_{x,y}\cdot\varphi_{x+1,y}) - \frac{1}{8\pi}\log(\varphi_{x,y}\cdot\varphi_{x-1,y}) \\ &-\frac{1}{8\pi}\log(\varphi_{x,y}\cdot\varphi_{x,y+1}) - \frac{1}{8\pi}\log(\varphi_{x,y}\cdot\varphi_{x,y-1}) + \frac{\mu^2}{4\pi}(1 - \varphi_{x,y}\cdot k) \end{aligned} \tag{8}$$

as a function of (x, y). Summing (8) over all lattice sites gives the total energy E.

Notice that the skyrmion in figure 1 is located at the centre of a lattice cell, which is also the centre of the whole lattice. If either n_x or n_y is odd, then in addition to the energy minimum, there also exists an unstable critical point of E. For example, if $n_x = n_y = 21$, then there is a skyrmion "balanced" on the lattice site at the centre (see figure 2). This has energy $E = 1.59888$, ie. 1% higher than the minimum. If $n_x = 21$ and $n_y = 22$, then there is an unstable skyrmion located at the middle of a link (figure 3). Its energy is $E = 1.59033$, which is 0.7% higher than the minimum. These energy differences represent the "Peierls-Nabarro potential". If we want to make the skyrmion move through the lattice, it has to have enough kinetic energy to overcome the potential barrier between adjacent lattice cells. Generally speaking, the skyrmion will lose energy as it moves, and eventually it gets pinned in one position. But this process may have a much longer time-scale than the dynamics one is investigating.

Finally, let us turn to the $N = 2$ case. If $n_x = n_y = 22$, the energy is minimized by the 2-skyrmion depicted in figure 4. It has a broader profile than the 1-skyrmion, but is still highly localized. Its energy is $E = 2.89439$, which is 8% lower than twice the energy of the 1-skyrmion. As before, there are also unstable critical points. If $n_x = n_y = 23$, we get an unstable 2-skyrmion centred at a lattice site (figure 5), with energy 2.92655 (again 1% above the minimum). Notice that the energy density is peaked not at the centre, but on a ring surrounding the centre; this is a well-known phenomenon in the continuum theory.

4. Concluding Remarks.

One application of the idea described above is that it may provide a highly efficient and economical way of modelling the continuum system. One should now study the dynamics of these lattice skyrmions, and in particular compare with numerical simulations of the continuum case [4,5]. There is of course a choice of dynamics: for example, it could be either dissipative or non-dissipative.

It is clear that this method extends to the actual Skyrme model, an O(4) sigma model in three spatial dimensions. Again, the Skyrme term will not appear explicitly in this lattice theory: its role will be taken by an appropriate choice of f. The details of this have yet to be investigated.

Is there a lattice version of the Bogomol'nyi bound (3)? For topological models in

one spatial dimension, there are lattice versions where the lower bound (3) exists and is saturated by static soliton solutions [13]. These have certain advantages, not least that the Peierls-Nabarro barrier is completely eliminated, and so a soliton can move freely through the lattice. But in higher dimensions, it seems to be much more difficult to find a lattice version of (3). So this remains an open question.

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